



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:13 AM GMT

PDB ID : 2G3M  
Title : Crystal structure of the Sulfolobus solfataricus alpha-glucosidase MalA  
Authors : Ernst, H.A.; Lo Leggio, L.; Willemoes, M.; Leonard, G.; Blum, P.; Larsen, S.  
Deposited on : 2006-02-20  
Resolution : 2.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

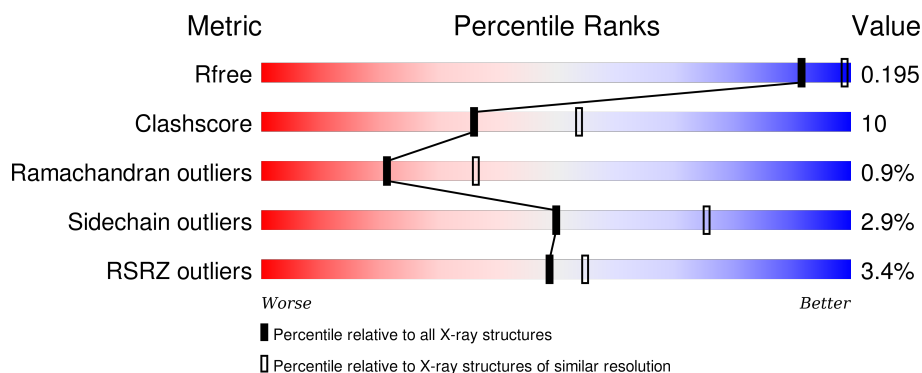
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	693	<div> <div>4%</div> <div>76%</div> <div>23%</div> <div>.</div> </div>
1	B	693	<div> <div>3%</div> <div>76%</div> <div>23%</div> <div>.</div> </div>
1	C	693	<div> <div>5%</div> <div>75%</div> <div>24%</div> <div>.</div> </div>
1	D	693	<div> <div>3%</div> <div>75%</div> <div>24%</div> <div>.</div> </div>
1	E	693	<div> <div>2%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	693	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a small red segment at the beginning labeled '4%', a large green segment in the middle labeled '76%', and a yellow segment at the end labeled '22%'. A small black dot is located at the far right end of the bar.

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 35378 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Alpha-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	691	Total	C	N	O	S	0	1	0
			5684	3703	919	1047	15			
1	B	691	Total	C	N	O	S	0	1	0
			5684	3703	919	1047	15			
1	C	691	Total	C	N	O	S	0	1	0
			5684	3703	919	1047	15			
1	D	691	Total	C	N	O	S	0	1	0
			5684	3703	919	1047	15			
1	E	691	Total	C	N	O	S	0	1	0
			5684	3703	919	1047	15			
1	F	692	Total	C	N	O	S	0	1	0
			5695	3709	923	1048	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	CLONING ARTIFACT	UNP O59645
A	2	ARG	-	CLONING ARTIFACT	UNP O59645
A	3	ILE	-	CLONING ARTIFACT	UNP O59645
A	4	LEU	-	CLONING ARTIFACT	UNP O59645
B	1	MET	-	CLONING ARTIFACT	UNP O59645
B	2	ARG	-	CLONING ARTIFACT	UNP O59645
B	3	ILE	-	CLONING ARTIFACT	UNP O59645
B	4	LEU	-	CLONING ARTIFACT	UNP O59645
C	1	MET	-	CLONING ARTIFACT	UNP O59645
C	2	ARG	-	CLONING ARTIFACT	UNP O59645
C	3	ILE	-	CLONING ARTIFACT	UNP O59645
C	4	LEU	-	CLONING ARTIFACT	UNP O59645
D	1	MET	-	CLONING ARTIFACT	UNP O59645
D	2	ARG	-	CLONING ARTIFACT	UNP O59645
D	3	ILE	-	CLONING ARTIFACT	UNP O59645
D	4	LEU	-	CLONING ARTIFACT	UNP O59645
E	1	MET	-	CLONING ARTIFACT	UNP O59645

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Chain	Residue	Modelled	Actual	Comment	Reference
E	2	ARG	-	CLONING ARTIFACT	UNP O59645
E	3	ILE	-	CLONING ARTIFACT	UNP O59645
E	4	LEU	-	CLONING ARTIFACT	UNP O59645
F	1	MET	-	CLONING ARTIFACT	UNP O59645
F	2	ARG	-	CLONING ARTIFACT	UNP O59645
F	3	ILE	-	CLONING ARTIFACT	UNP O59645
F	4	LEU	-	CLONING ARTIFACT	UNP O59645

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	213	Total O 213 213	0	0
2	B	210	Total O 210 210	0	0
2	C	178	Total O 178 178	0	0
2	D	221	Total O 221 221	0	0
2	E	249	Total O 249 249	0	0
2	F	192	Total O 192 192	0	0

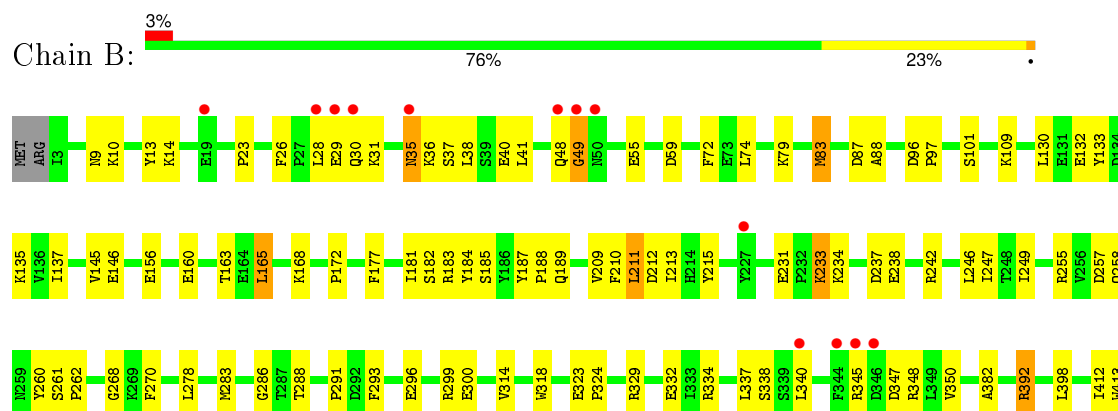
### 3 Residue-property plots

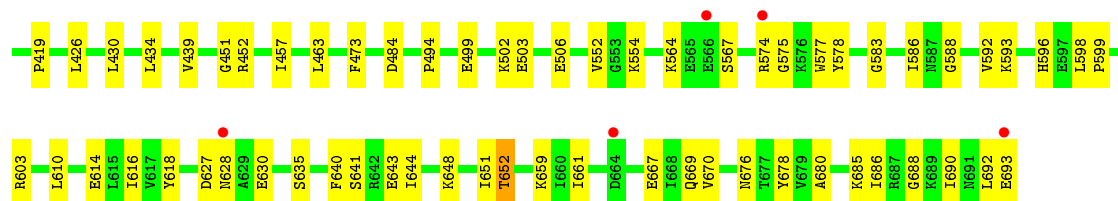
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Alpha-glucosidase

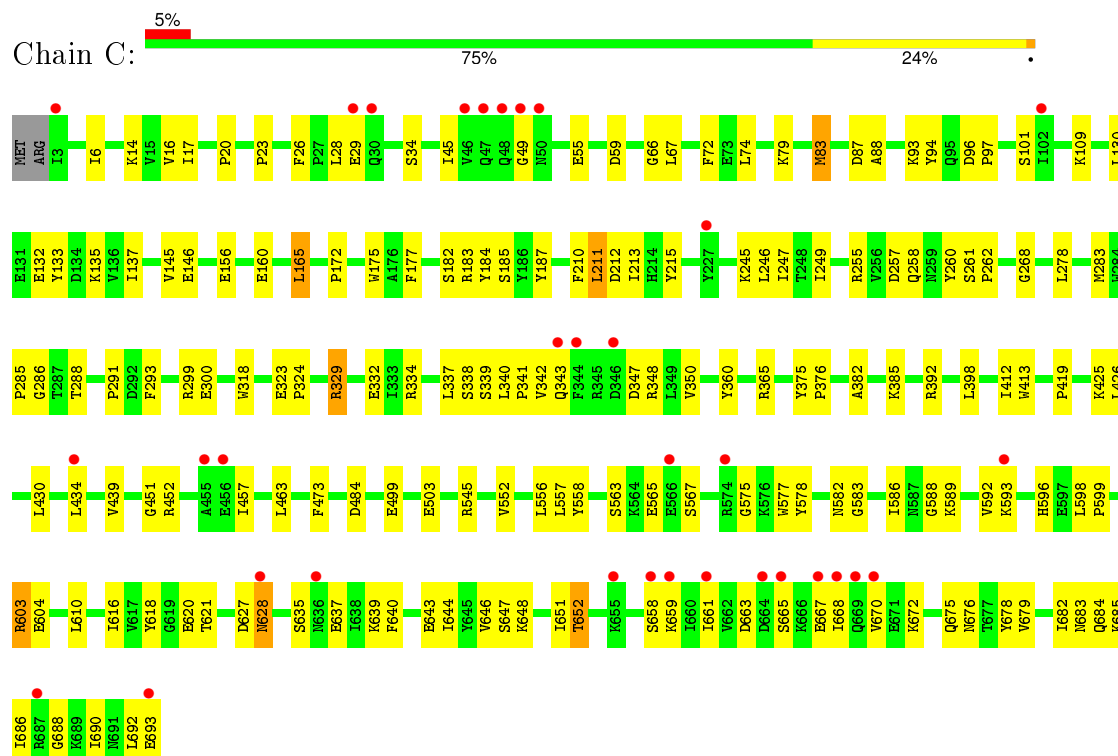


#### • Molecule 1: Alpha-glucosidase

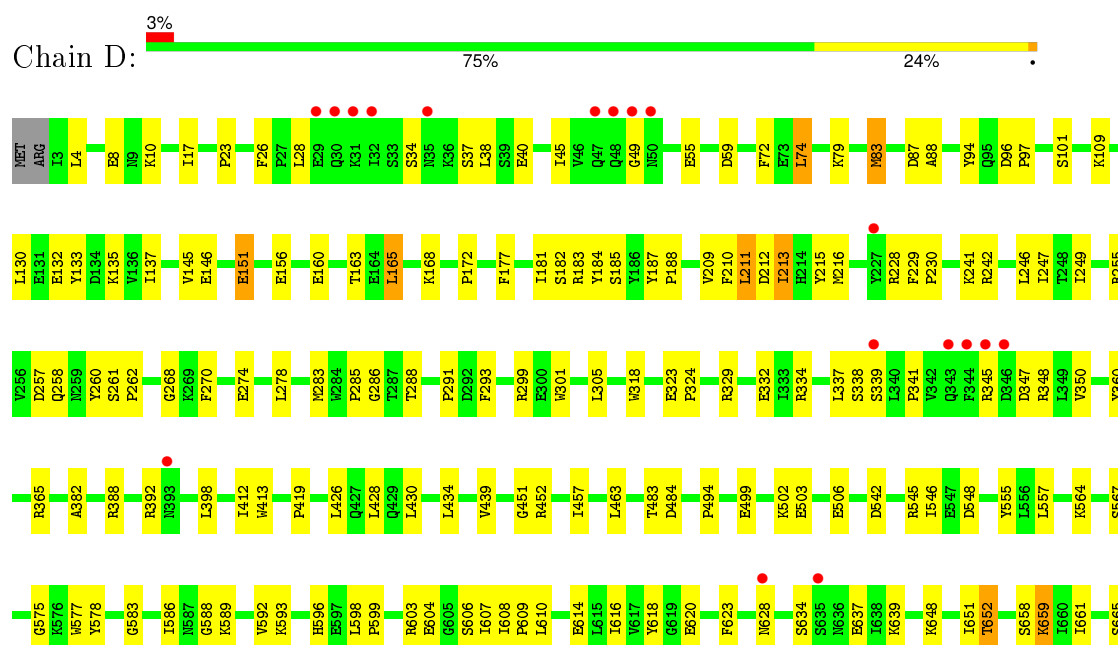


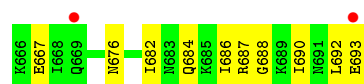


• Molecule 1: Alpha-glucosidase

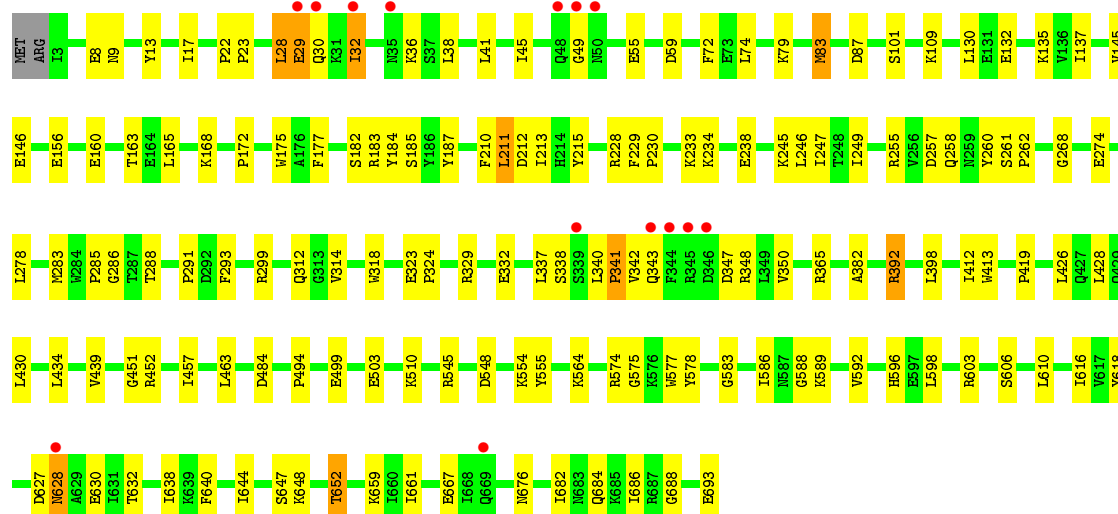
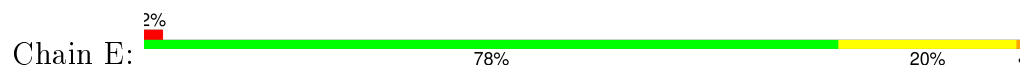


• Molecule 1: Alpha-glucosidase

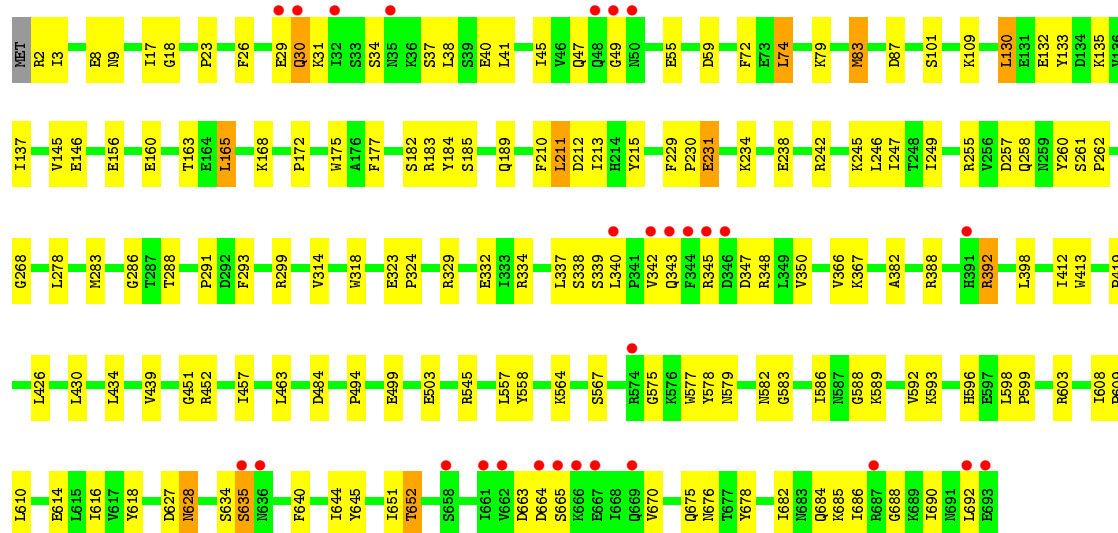
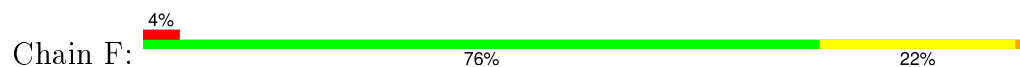




● Molecule 1: Alpha-glucosidase



● Molecule 1: Alpha-glucosidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.17Å 173.56Å 154.08Å 90.00° 108.00° 90.00°	Depositor
Resolution (Å)	34.25 – 2.55 34.25 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.25-2.55) 100.0 (34.25-2.55)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.95 (at 2.54Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.170 , 0.195 0.171 , 0.195	Depositor DCC
$R_{free}$ test set	8380 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.7	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 41.6	EDS
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 167412 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	35378	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.36	0/5838	0.61	0/7902
1	B	0.36	0/5838	0.61	0/7902
1	C	0.36	0/5838	0.60	0/7902
1	D	0.37	0/5838	0.61	0/7902
1	E	0.37	0/5838	0.62	0/7902
1	F	0.36	0/5849	0.61	0/7916
All	All	0.36	0/35039	0.61	0/47426

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5684	0	5651	109	0
1	B	5684	0	5651	115	0
1	C	5684	0	5651	125	0
1	D	5684	0	5651	127	0
1	E	5684	0	5651	111	0
1	F	5695	0	5664	123	0
2	A	213	0	0	2	0
2	B	210	0	0	3	0
2	C	178	0	0	2	0
2	D	221	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	249	0	0	4	0
2	F	192	0	0	4	0
All	All	35378	0	33919	651	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (651) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:661:ILE:HG12	1:D:667:GLU:HG2	1.41	1.02
1:A:258:GLN:HG3	1:E:278:LEU:HD21	1.51	0.93
1:D:564:LYS:H	1:D:564:LYS:HD2	1.31	0.91
1:B:564:LYS:H	1:B:564:LYS:HD2	1.37	0.88
1:B:35:ASN:H	1:B:35:ASN:HD22	1.23	0.85
1:B:258:GLN:HG3	1:D:278:LEU:HD21	1.58	0.85
1:E:163:THR:HG22	1:E:168:LYS:HD3	1.57	0.83
1:C:686:ILE:HD13	1:C:690:ILE:HD11	1.57	0.83
1:C:278:LEU:HD21	1:F:258:GLN:HG3	1.58	0.83
1:C:299:ARG:HG3	1:C:382:ALA:HB2	1.60	0.82
1:C:596:HIS:HD2	1:C:598:LEU:H	1.26	0.82
1:C:332:GLU:HG3	1:F:332:GLU:HG3	1.60	0.81
1:A:686:ILE:HD13	1:A:690:ILE:HD11	1.63	0.81
1:D:341:PRO:HA	1:F:345:ARG:NH1	1.97	0.80
1:E:577:TRP:CZ3	1:E:603:ARG:HB3	2.16	0.79
1:B:278:LEU:HD21	1:D:258:GLN:HG3	1.61	0.79
1:A:670:VAL:CG1	1:A:678:TYR:HB3	2.11	0.79
1:D:651:ILE:HD13	1:D:692:LEU:HD21	1.65	0.78
1:C:299:ARG:CG	1:C:382:ALA:HB2	2.14	0.78
1:D:299:ARG:HG3	1:D:382:ALA:HB2	1.66	0.78
1:A:610:LEU:HD11	1:A:616:ILE:HD11	1.66	0.77
1:A:163:THR:HG22	1:A:168:LYS:HD3	1.67	0.77
1:B:564:LYS:N	1:B:564:LYS:HD2	1.98	0.77
1:E:299:ARG:HG3	1:E:382:ALA:HB2	1.66	0.77
1:F:163:THR:HG22	1:F:168:LYS:HD3	1.68	0.76
1:C:596:HIS:CD2	1:C:598:LEU:H	2.02	0.76
1:D:618:TYR:HB2	1:D:652:THR:HG23	1.66	0.76
1:F:8:GLU:HB2	1:F:34:SER:HB2	1.68	0.75
1:D:163:THR:HG22	1:D:168:LYS:HD3	1.69	0.75
1:D:564:LYS:HD2	1:D:564:LYS:N	2.02	0.75
1:E:163:THR:CG2	1:E:168:LYS:HD3	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:596:HIS:HD2	1:F:598:LEU:H	1.35	0.74
1:B:314:VAL:O	1:B:392:ARG:NH2	2.20	0.74
1:B:35:ASN:H	1:B:35:ASN:ND2	1.86	0.73
1:B:347:ASP:O	1:B:350:VAL:HG12	1.89	0.73
1:B:299:ARG:HG2	1:B:382:ALA:HB2	1.70	0.73
1:C:567:SER:OG	1:C:593:LYS:HE3	1.89	0.73
1:F:37:SER:OG	1:F:40:GLU:HG3	1.88	0.73
1:B:299:ARG:CG	1:B:382:ALA:HB2	2.19	0.72
1:E:596:HIS:HD2	1:E:598:LEU:H	1.37	0.72
1:B:37:SER:OG	1:B:40:GLU:HG3	1.89	0.72
1:E:299:ARG:CG	1:E:382:ALA:HB2	2.18	0.72
1:E:38:LEU:HD21	1:E:45:ILE:HD12	1.71	0.72
1:F:596:HIS:CD2	1:F:598:LEU:H	2.08	0.72
1:B:651:ILE:HD13	1:B:692:LEU:HD21	1.72	0.72
1:B:596:HIS:HD2	1:B:598:LEU:H	1.36	0.71
1:A:686:ILE:CD1	1:A:690:ILE:HD11	2.20	0.71
1:B:36:LYS:HE3	2:B:896:HOH:O	1.89	0.71
1:D:686:ILE:HD13	1:D:690:ILE:HD11	1.72	0.71
1:C:618:TYR:HB2	1:C:652:THR:HG23	1.71	0.70
1:A:258:GLN:CG	1:E:278:LEU:HD21	2.19	0.70
1:C:258:GLN:HG3	1:F:278:LEU:HD21	1.71	0.70
1:B:686:ILE:HD13	1:B:690:ILE:HD11	1.72	0.70
1:A:670:VAL:HG11	1:A:678:TYR:HB3	1.71	0.70
1:C:425:LYS:HG3	2:C:832:HOH:O	1.92	0.70
1:D:299:ARG:CG	1:D:382:ALA:HB2	2.22	0.69
1:A:286:GLY:O	1:A:288:THR:HG23	1.93	0.69
1:A:8:GLU:O	1:A:30:GLN:HG3	1.93	0.69
1:C:17:ILE:HD11	1:C:45:ILE:HD13	1.74	0.69
1:E:13:TYR:CE2	1:E:36:LYS:HG3	2.27	0.69
1:B:268:GLY:H	1:D:258:GLN:HG2	1.59	0.68
1:C:286:GLY:O	1:C:288:THR:HG23	1.94	0.68
1:A:630:GLU:HB2	1:A:641:SER:HB3	1.76	0.68
1:F:299:ARG:CG	1:F:382:ALA:HB2	2.24	0.68
1:F:610:LEU:HD11	1:F:616:ILE:HD11	1.74	0.67
1:B:233:LYS:HE3	1:B:237:ASP:OD2	1.94	0.67
1:A:314:VAL:O	1:A:392:ARG:NH2	2.28	0.67
1:B:286:GLY:O	1:B:288:THR:HG23	1.94	0.67
1:C:278:LEU:HD21	1:F:258:GLN:CG	2.25	0.67
1:B:14:LYS:HD2	1:B:28:LEU:HD12	1.76	0.67
1:A:278:LEU:HD21	1:E:258:GLN:HG3	1.76	0.67
1:B:185:SER:OG	1:B:212:ASP:HB3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:646:VAL:HG21	1:C:686:ILE:HD12	1.77	0.67
1:D:286:GLY:O	1:D:288:THR:HG23	1.95	0.67
1:A:567:SER:OG	1:A:593:LYS:HE3	1.95	0.66
1:E:286:GLY:O	1:E:288:THR:HG23	1.95	0.66
1:C:563:SER:OG	1:C:565:GLU:HG2	1.95	0.66
1:B:258:GLN:HG2	1:D:268:GLY:H	1.60	0.66
1:B:258:GLN:CG	1:D:278:LEU:HD21	2.23	0.66
1:F:38:LEU:HD21	1:F:45:ILE:HD12	1.76	0.66
1:E:314:VAL:O	1:E:392:ARG:NH2	2.29	0.66
1:F:286:GLY:O	1:F:288:THR:HG23	1.96	0.66
1:D:577:TRP:CZ3	1:D:603:ARG:HB3	2.31	0.66
1:F:686:ILE:CD1	1:F:690:ILE:HD11	2.27	0.65
1:C:337:LEU:HD21	1:F:337:LEU:HD21	1.76	0.65
1:C:185:SER:OG	1:C:212:ASP:HB3	1.95	0.65
1:B:278:LEU:HD21	1:D:258:GLN:CG	2.27	0.65
1:A:185:SER:OG	1:A:212:ASP:HB3	1.96	0.65
1:E:185:SER:OG	1:E:212:ASP:HB3	1.97	0.65
1:F:185:SER:OG	1:F:212:ASP:HB3	1.97	0.65
1:A:452:ARG:HD3	1:A:484:ASP:O	1.97	0.65
1:E:30:GLN:O	1:E:32:ILE:HG22	1.97	0.65
1:F:651:ILE:HD13	1:F:692:LEU:HD21	1.78	0.65
1:D:564:LYS:CD	1:D:564:LYS:H	2.08	0.64
1:A:163:THR:CG2	1:A:168:LYS:HD3	2.26	0.64
1:D:185:SER:OG	1:D:212:ASP:HB3	1.96	0.64
1:F:682:ILE:HG22	1:F:684:GLN:HG2	1.80	0.64
1:B:334:ARG:O	1:B:338:SER:HB2	1.98	0.64
1:B:337:LEU:HD21	1:D:337:LEU:HD21	1.79	0.64
1:F:23:PRO:HG3	2:F:722:HOH:O	1.97	0.63
1:B:564:LYS:H	1:B:564:LYS:CD	2.11	0.63
1:C:258:GLN:HG2	1:F:268:GLY:H	1.63	0.63
1:C:23:PRO:HG3	2:C:722:HOH:O	1.98	0.63
1:C:332:GLU:CG	1:F:332:GLU:HG3	2.28	0.63
1:E:452:ARG:HD3	1:E:484:ASP:O	1.99	0.63
1:B:452:ARG:HD3	1:B:484:ASP:O	1.99	0.63
1:F:452:ARG:HD3	1:F:484:ASP:O	1.98	0.63
1:F:567:SER:OG	1:F:593:LYS:HE3	1.98	0.63
1:E:554:LYS:O	1:E:603:ARG:HD3	1.99	0.63
1:A:577:TRP:CZ3	1:A:603:ARG:HB3	2.33	0.63
1:B:23:PRO:HG3	2:B:722:HOH:O	1.99	0.63
1:D:452:ARG:HD3	1:D:484:ASP:O	1.97	0.63
1:F:610:LEU:HB2	1:F:614:GLU:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:ARG:HD3	2:B:876:HOH:O	1.99	0.63
1:B:577:TRP:CZ3	1:B:603:ARG:HB3	2.34	0.63
1:F:575:GLY:O	1:F:588:GLY:N	2.33	0.62
1:A:596:HIS:HD2	1:A:598:LEU:H	1.46	0.62
1:F:618:TYR:HB2	1:F:652:THR:HG23	1.80	0.62
1:C:339:SER:HB3	1:D:339:SER:CB	2.29	0.62
1:A:261:SER:HB3	1:A:262:PRO:HD3	1.81	0.62
1:C:452:ARG:HD3	1:C:484:ASP:O	1.99	0.62
1:D:87:ASP:O	1:D:348:ARG:HD3	2.00	0.62
1:F:686:ILE:HD13	1:F:690:ILE:HD11	1.82	0.62
1:B:87:ASP:O	1:B:348:ARG:HD3	2.00	0.62
1:D:323:GLU:N	1:D:324:PRO:HA	2.15	0.62
1:B:163:THR:HG22	1:B:168:LYS:HD3	1.82	0.61
1:A:299:ARG:CG	1:A:382:ALA:HB2	2.29	0.61
1:E:574:ARG:HD3	2:E:893:HOH:O	2.00	0.61
1:F:87:ASP:O	1:F:348:ARG:HD3	2.00	0.61
1:F:299:ARG:HG2	1:F:382:ALA:HB2	1.81	0.61
1:F:17:ILE:HD11	1:F:45:ILE:HD13	1.83	0.61
1:C:683:ASN:H	1:C:683:ASN:HD22	1.47	0.61
1:D:23:PRO:HG3	2:D:721:HOH:O	2.00	0.61
1:B:596:HIS:CD2	1:B:598:LEU:H	2.17	0.61
1:F:261:SER:HB3	1:F:262:PRO:HD3	1.82	0.61
1:B:55:GLU:HG2	1:B:137:ILE:HG12	1.82	0.61
1:C:261:SER:HB3	1:C:262:PRO:HD3	1.83	0.61
1:C:627:ASP:O	1:C:628:ASN:HB3	1.99	0.61
1:B:261:SER:HB3	1:B:262:PRO:HD3	1.82	0.60
1:C:26:PHE:HB3	1:C:165:LEU:HD22	1.83	0.60
1:A:661:ILE:HG12	1:A:667:GLU:HG2	1.83	0.60
1:C:668:ILE:HD13	1:C:682:ILE:HA	1.83	0.60
1:B:578:TYR:CE1	1:B:583:GLY:HA2	2.36	0.60
1:B:9:ASN:ND2	1:B:10:LYS:HG3	2.15	0.60
1:E:323:GLU:N	1:E:324:PRO:HA	2.16	0.60
1:D:261:SER:HB3	1:D:262:PRO:HD3	1.83	0.60
1:F:340:LEU:HB3	1:F:342:VAL:HG12	1.83	0.60
1:E:575:GLY:O	1:E:588:GLY:N	2.34	0.60
1:E:23:PRO:HG3	2:E:723:HOH:O	2.01	0.60
1:C:618:TYR:HB2	1:C:652:THR:CG2	2.31	0.60
1:D:575:GLY:O	1:D:588:GLY:N	2.33	0.60
1:F:347:ASP:O	1:F:350:VAL:HG12	2.02	0.60
1:A:330:ALA:O	1:A:334:ARG:HG2	2.02	0.60
1:F:323:GLU:N	1:F:324:PRO:HA	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:683:ASN:N	1:C:683:ASN:HD22	1.98	0.60
1:A:23:PRO:HG3	2:A:720:HOH:O	2.01	0.60
1:A:596:HIS:CD2	1:A:598:LEU:H	2.20	0.60
1:B:575:GLY:O	1:B:588:GLY:N	2.35	0.60
1:B:323:GLU:N	1:B:324:PRO:HA	2.17	0.59
1:C:575:GLY:O	1:C:588:GLY:N	2.33	0.59
1:A:17:ILE:HD11	1:A:45:ILE:HD13	1.84	0.59
1:C:268:GLY:H	1:F:258:GLN:HG2	1.67	0.59
1:B:26:PHE:HB3	1:B:165:LEU:HD22	1.83	0.59
1:D:607:ILE:C	1:D:608:ILE:HD12	2.23	0.59
1:A:323:GLU:N	1:A:324:PRO:HA	2.17	0.59
1:E:596:HIS:CD2	1:E:598:LEU:H	2.20	0.59
1:C:334:ARG:O	1:C:338:SER:HB2	2.02	0.59
1:E:55:GLU:HG2	1:E:137:ILE:HG12	1.85	0.59
1:C:323:GLU:N	1:C:324:PRO:HA	2.17	0.59
1:F:577:TRP:CZ3	1:F:603:ARG:HB3	2.38	0.59
1:D:132:GLU:HG3	2:D:832:HOH:O	2.03	0.58
1:E:618:TYR:HB2	1:E:652:THR:HG23	1.86	0.58
1:A:575:GLY:O	1:A:588:GLY:N	2.34	0.58
1:A:339:SER:HB2	1:F:339:SER:HB3	1.84	0.58
1:C:557:LEU:C	1:C:557:LEU:HD23	2.23	0.58
1:B:643:GLU:OE2	1:B:685:LYS:HD3	2.03	0.58
1:B:268:GLY:N	1:D:258:GLN:HG2	2.19	0.58
1:F:557:LEU:HD23	1:F:558:TYR:N	2.17	0.58
1:B:340:LEU:HD11	1:E:340:LEU:HD13	1.85	0.58
1:C:686:ILE:CD1	1:C:690:ILE:HD11	2.29	0.58
1:D:614:GLU:HG2	1:D:648:LYS:HB3	1.83	0.58
1:D:55:GLU:HG2	1:D:137:ILE:HG12	1.86	0.58
1:A:87:ASP:O	1:A:348:ARG:HD3	2.04	0.58
1:E:261:SER:HB3	1:E:262:PRO:HD3	1.86	0.58
1:B:618:TYR:HB2	1:B:652:THR:HG23	1.84	0.58
1:A:419:PRO:HG2	1:A:457:ILE:HG23	1.85	0.58
1:D:499:GLU:O	1:D:503:GLU:HG3	2.04	0.58
1:F:412:ILE:HD12	1:F:439:VAL:HG11	1.87	0.57
1:F:55:GLU:HG2	1:F:137:ILE:HG12	1.86	0.57
1:B:35:ASN:HD22	1:B:35:ASN:N	1.91	0.57
1:E:419:PRO:HG2	1:E:457:ILE:HG23	1.87	0.57
1:C:87:ASP:O	1:C:348:ARG:HD3	2.04	0.57
1:E:8:GLU:O	1:E:32:ILE:HG23	2.04	0.57
1:B:499:GLU:O	1:B:503:GLU:HG3	2.05	0.57
1:D:26:PHE:HB3	1:D:165:LEU:HD22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:LEU:HD21	1:E:337:LEU:HD21	1.87	0.57
1:D:686:ILE:CD1	1:D:690:ILE:HD11	2.35	0.57
1:E:661:ILE:CD1	1:E:693:GLU:HG3	2.35	0.57
1:A:55:GLU:HG2	1:A:137:ILE:HG12	1.86	0.57
1:C:258:GLN:HG2	1:F:268:GLY:N	2.19	0.57
1:F:618:TYR:HB2	1:F:652:THR:CG2	2.35	0.57
1:C:14:LYS:HD2	1:C:28:LEU:HD12	1.87	0.56
1:D:659:LYS:HB3	1:D:659:LYS:NZ	2.20	0.56
1:D:360:TYR:CZ	1:D:365:ARG:HD2	2.40	0.56
1:B:258:GLN:HG2	1:D:268:GLY:N	2.20	0.56
1:B:255:ARG:HG2	1:B:257:ASP:HB2	1.87	0.56
1:F:293:PHE:O	1:F:299:ARG:HD3	2.05	0.56
1:A:255:ARG:HG2	1:A:257:ASP:HB2	1.87	0.56
1:C:156:GLU:O	1:C:160:GLU:HG3	2.05	0.56
1:C:55:GLU:HG2	1:C:137:ILE:HG12	1.86	0.56
1:C:347:ASP:O	1:C:350:VAL:HG12	2.05	0.56
1:A:412:ILE:HD12	1:A:439:VAL:HG11	1.87	0.56
1:F:156:GLU:O	1:F:160:GLU:HG3	2.06	0.56
1:E:59:ASP:OD2	1:E:109:LYS:HD2	2.06	0.56
1:E:342:VAL:CG1	1:F:342:VAL:HG23	2.36	0.55
1:F:342:VAL:HG22	1:F:343:GLN:N	2.21	0.55
1:C:419:PRO:HG2	1:C:457:ILE:HG23	1.88	0.55
1:D:255:ARG:HG2	1:D:257:ASP:HB2	1.88	0.55
1:E:610:LEU:HD11	1:E:616:ILE:HD11	1.88	0.55
1:F:255:ARG:HG2	1:F:257:ASP:HB2	1.88	0.55
1:F:499:GLU:O	1:F:503:GLU:HG3	2.07	0.55
1:E:156:GLU:O	1:E:160:GLU:HG3	2.06	0.55
1:B:59:ASP:OD2	1:B:109:LYS:HD2	2.06	0.55
1:A:643:GLU:OE2	1:A:685:LYS:HD2	2.06	0.55
1:D:618:TYR:HB2	1:D:652:THR:CG2	2.34	0.55
1:B:412:ILE:HD12	1:B:439:VAL:HG11	1.88	0.55
1:F:419:PRO:HG2	1:F:457:ILE:HG23	1.88	0.55
1:D:163:THR:CG2	1:D:168:LYS:HD3	2.37	0.55
1:D:419:PRO:HG2	1:D:457:ILE:HG23	1.87	0.55
1:C:255:ARG:HG2	1:C:257:ASP:HB2	1.87	0.55
1:A:156:GLU:O	1:A:160:GLU:HG3	2.06	0.55
1:D:578:TYR:CE1	1:D:583:GLY:HA2	2.42	0.55
1:D:334:ARG:O	1:D:338:SER:HB2	2.07	0.55
1:C:651:ILE:HD13	1:C:692:LEU:HD21	1.89	0.55
1:B:614:GLU:HG2	1:B:648:LYS:HB3	1.87	0.55
1:E:234:LYS:O	1:E:238:GLU:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:GLU:O	1:D:160:GLU:HG3	2.07	0.55
1:D:637:GLU:OE2	1:D:639:LYS:HE3	2.08	0.54
1:B:661:ILE:HG12	1:B:667:GLU:HG2	1.88	0.54
1:B:419:PRO:HG2	1:B:457:ILE:HG23	1.88	0.54
1:C:59:ASP:OD2	1:C:109:LYS:HD2	2.07	0.54
1:C:299:ARG:HG2	1:C:382:ALA:HB2	1.90	0.54
1:F:334:ARG:O	1:F:338:SER:HB3	2.06	0.54
1:F:675:GLN:HG2	1:F:676:ASN:ND2	2.23	0.54
1:D:59:ASP:OD2	1:D:109:LYS:HD2	2.07	0.54
1:F:59:ASP:OD2	1:F:109:LYS:HD2	2.07	0.54
1:E:87:ASP:O	1:E:348:ARG:HD3	2.08	0.54
1:E:412:ILE:HD12	1:E:439:VAL:HG11	1.89	0.54
1:F:132:GLU:HG3	2:F:826:HOH:O	2.07	0.54
1:E:342:VAL:HG11	1:F:342:VAL:HG23	1.89	0.54
1:A:618:TYR:HB2	1:A:652:THR:HG23	1.90	0.54
1:C:577:TRP:CZ3	1:C:603:ARG:HB3	2.42	0.54
1:F:163:THR:CG2	1:F:168:LYS:HD3	2.35	0.54
1:E:342:VAL:HG12	1:E:343:GLN:N	2.22	0.54
1:E:578:TYR:CE1	1:E:583:GLY:HA2	2.43	0.54
1:A:299:ARG:HG3	1:A:382:ALA:HB2	1.90	0.54
1:E:255:ARG:HG2	1:E:257:ASP:HB2	1.89	0.53
1:D:652:THR:HA	1:D:676:ASN:O	2.08	0.53
1:E:682:ILE:HG22	1:E:684:GLN:HG2	1.91	0.53
1:E:577:TRP:CH2	1:E:603:ARG:HB3	2.43	0.53
1:C:682:ILE:HG22	1:C:684:GLN:HG2	1.91	0.53
1:B:651:ILE:HD13	1:B:692:LEU:CD2	2.38	0.53
1:E:659:LYS:HD2	1:E:667:GLU:HG3	1.90	0.53
1:A:652:THR:HA	1:A:676:ASN:O	2.09	0.53
1:D:83:MET:HG3	1:D:101:SER:HB3	1.91	0.53
1:C:499:GLU:O	1:C:503:GLU:HG3	2.08	0.53
1:A:59:ASP:OD2	1:A:109:LYS:HD2	2.08	0.53
1:D:412:ILE:HD12	1:D:439:VAL:HG11	1.89	0.53
1:B:299:ARG:HG3	1:B:382:ALA:HB2	1.91	0.53
1:A:268:GLY:H	1:E:258:GLN:HG2	1.74	0.53
1:B:652:THR:HA	1:B:676:ASN:O	2.09	0.53
1:C:182:SER:HB2	1:C:210:PHE:HB2	1.91	0.52
1:B:234:LYS:O	1:B:238:GLU:HG3	2.09	0.52
1:A:334:ARG:O	1:A:338:SER:HB3	2.09	0.52
1:C:412:ILE:HD12	1:C:439:VAL:HG11	1.89	0.52
1:D:596:HIS:CD2	1:D:598:LEU:H	2.27	0.52
1:B:156:GLU:O	1:B:160:GLU:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:182:SER:HB2	1:F:210:PHE:HB2	1.92	0.52
1:C:652:THR:HA	1:C:676:ASN:O	2.10	0.52
1:C:578:TYR:CE1	1:C:583:GLY:HA2	2.44	0.52
1:D:388:ARG:HD3	2:D:850:HOH:O	2.08	0.52
1:D:651:ILE:HD13	1:D:692:LEU:CD2	2.38	0.52
1:D:10:LYS:HG2	1:D:10:LYS:O	2.10	0.52
1:C:17:ILE:HD11	1:C:45:ILE:CD1	2.39	0.52
1:F:234:LYS:O	1:F:238:GLU:HG3	2.09	0.52
1:F:299:ARG:HG3	1:F:382:ALA:HB2	1.90	0.52
1:E:342:VAL:CG1	1:E:343:GLN:N	2.73	0.52
1:A:274:GLU:O	1:A:365:ARG:NH2	2.43	0.52
1:A:586:ILE:HD13	1:A:592:VAL:HG11	1.92	0.51
1:C:258:GLN:CG	1:F:278:LEU:HD21	2.38	0.51
1:A:268:GLY:N	1:E:258:GLN:HG2	2.25	0.51
1:A:557:LEU:HD23	1:A:557:LEU:C	2.30	0.51
1:D:293:PHE:O	1:D:299:ARG:HD3	2.10	0.51
1:A:554:LYS:O	1:A:603:ARG:HD3	2.11	0.51
1:B:163:THR:CG2	1:B:168:LYS:HD3	2.41	0.51
1:B:35:ASN:ND2	1:B:35:ASN:N	2.51	0.51
1:E:274:GLU:O	1:E:365:ARG:NH2	2.38	0.51
1:B:340:LEU:CD1	1:E:340:LEU:HD13	2.41	0.51
1:C:6:ILE:HG22	1:C:34:SER:HB2	1.92	0.51
1:E:652:THR:HA	1:E:676:ASN:O	2.11	0.51
1:A:499:GLU:O	1:A:503:GLU:HG3	2.11	0.51
1:D:586:ILE:HD13	1:D:592:VAL:HG11	1.93	0.51
1:A:679:VAL:HG12	1:A:680:ALA:N	2.26	0.51
1:A:299:ARG:HG2	1:A:382:ALA:HB2	1.91	0.51
1:C:268:GLY:N	1:F:258:GLN:HG2	2.26	0.50
1:E:182:SER:HB2	1:E:210:PHE:HB2	1.93	0.50
1:B:172:PRO:HG2	1:B:177:PHE:CE1	2.46	0.50
1:A:578:TYR:CE1	1:A:583:GLY:HA2	2.46	0.50
1:A:132:GLU:HG3	2:A:835:HOH:O	2.11	0.50
1:B:72:PHE:CZ	1:B:79:LYS:HE2	2.46	0.50
1:C:675:GLN:HG2	1:C:676:ASN:ND2	2.26	0.50
1:E:640:PHE:CE2	1:E:644:ILE:HD11	2.46	0.50
1:D:72:PHE:CZ	1:D:79:LYS:HE2	2.47	0.50
1:A:132:GLU:HB3	1:A:135:LYS:HB2	1.93	0.50
1:F:586:ILE:HD13	1:F:592:VAL:HG11	1.94	0.50
1:C:291:PRO:HG2	1:C:293:PHE:CE2	2.46	0.50
1:D:341:PRO:HA	1:F:345:ARG:HH12	1.75	0.50
1:A:293:PHE:O	1:A:299:ARG:HD3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:LYS:HA	1:A:670:VAL:HG23	1.93	0.50
1:B:692:LEU:HD12	1:B:692:LEU:N	2.27	0.50
1:B:686:ILE:CD1	1:B:690:ILE:HD11	2.39	0.50
1:F:291:PRO:HG2	1:F:293:PHE:CE2	2.47	0.50
1:D:682:ILE:HG22	1:D:684:GLN:HG2	1.94	0.50
1:D:229:PHE:N	1:D:230:PRO:HD3	2.25	0.50
1:E:347:ASP:O	1:E:350:VAL:HG12	2.11	0.50
1:D:172:PRO:HG2	1:D:177:PHE:CE1	2.47	0.50
1:A:211:LEU:HD22	1:A:246:LEU:HD11	1.93	0.50
1:C:211:LEU:HD22	1:C:246:LEU:HD11	1.94	0.50
1:A:172:PRO:HG2	1:A:177:PHE:CE1	2.46	0.50
1:E:72:PHE:CZ	1:E:79:LYS:HE2	2.47	0.50
1:E:229:PHE:N	1:E:230:PRO:HD3	2.26	0.50
1:E:564:LYS:N	1:E:564:LYS:HD2	2.27	0.50
1:B:586:ILE:HD13	1:B:592:VAL:HG11	1.94	0.50
1:A:339:SER:HB2	1:F:339:SER:CB	2.41	0.50
1:B:293:PHE:O	1:B:299:ARG:HD3	2.12	0.49
1:A:83:MET:HG3	1:A:101:SER:HB3	1.93	0.49
1:D:181:ILE:CG1	1:D:209:VAL:HG12	2.41	0.49
1:B:627:ASP:O	1:B:628:ASN:CG	2.51	0.49
1:C:586:ILE:HD13	1:C:592:VAL:HG11	1.94	0.49
1:A:291:PRO:HG2	1:A:293:PHE:CE2	2.47	0.49
1:F:257:ASP:HB3	1:F:260:TYR:CB	2.42	0.49
1:C:648:LYS:HD2	1:C:679:VAL:HG11	1.94	0.49
1:A:682:ILE:HG22	1:A:684:GLN:HG2	1.94	0.49
1:A:72:PHE:CZ	1:A:79:LYS:HE2	2.48	0.49
1:C:451:GLY:O	1:C:452:ARG:HG3	2.12	0.49
1:C:72:PHE:CZ	1:C:79:LYS:HE2	2.48	0.49
1:C:172:PRO:HG2	1:C:177:PHE:CE1	2.48	0.49
1:B:554:LYS:O	1:B:603:ARG:HD3	2.13	0.49
1:E:586:ILE:HD13	1:E:592:VAL:HG11	1.94	0.49
1:C:683:ASN:N	1:C:683:ASN:ND2	2.60	0.49
1:C:83:MET:HG3	1:C:101:SER:HB3	1.94	0.49
1:E:291:PRO:HG2	1:E:293:PHE:CE2	2.48	0.49
1:F:610:LEU:HD11	1:F:616:ILE:CD1	2.43	0.49
1:F:132:GLU:HB3	1:F:135:LYS:HB2	1.95	0.49
1:F:72:PHE:CZ	1:F:79:LYS:HE2	2.47	0.49
1:D:257:ASP:HB3	1:D:260:TYR:CB	2.43	0.49
1:B:610:LEU:HD11	1:B:616:ILE:HD11	1.95	0.48
1:E:132:GLU:HB3	1:E:135:LYS:HB2	1.95	0.48
1:D:291:PRO:HG2	1:D:293:PHE:CE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:PRO:HG2	1:B:293:PHE:CE2	2.47	0.48
1:B:257:ASP:HB3	1:B:260:TYR:CB	2.42	0.48
1:E:659:LYS:HD2	1:E:667:GLU:CG	2.43	0.48
1:E:392:ARG:NH1	2:E:905:HOH:O	2.46	0.48
1:E:564:LYS:H	1:E:564:LYS:HD2	1.77	0.48
1:D:301:TRP:CZ2	1:D:305:LEU:HD11	2.48	0.48
1:D:133:TYR:HB3	1:E:187:TYR:O	2.12	0.48
1:A:556:LEU:HD23	1:A:557:LEU:N	2.28	0.48
1:E:312:GLN:HG2	2:E:929:HOH:O	2.12	0.48
1:C:300:GLU:HG2	1:C:385:LYS:NZ	2.29	0.48
1:B:211:LEU:HD22	1:B:246:LEU:HD11	1.95	0.48
1:D:545:ARG:HB2	1:E:494:PRO:HG3	1.96	0.48
1:A:589:LYS:HA	1:A:589:LYS:HD2	1.67	0.48
1:E:172:PRO:HG2	1:E:177:PHE:CE1	2.49	0.48
1:B:567:SER:OG	1:B:593:LYS:HE3	2.12	0.48
1:F:17:ILE:HD11	1:F:45:ILE:CD1	2.43	0.48
1:E:83:MET:HG3	1:E:101:SER:HB3	1.94	0.48
1:E:499:GLU:O	1:E:503:GLU:HG3	2.13	0.48
1:B:181:ILE:CG1	1:B:209:VAL:HG12	2.43	0.48
1:B:13:TYR:OH	1:B:36:LYS:HD2	2.13	0.48
1:F:172:PRO:HG2	1:F:177:PHE:CE1	2.48	0.48
1:F:189:GLN:HE22	1:F:231:GLU:HB2	1.78	0.48
1:E:211:LEU:HD22	1:E:246:LEU:HD11	1.95	0.48
1:E:247:ILE:N	1:E:247:ILE:HD12	2.29	0.48
1:C:659:LYS:HA	1:C:670:VAL:HG23	1.96	0.48
1:E:661:ILE:HD13	1:E:693:GLU:HG3	1.96	0.48
1:B:630:GLU:HB2	1:B:641:SER:HB3	1.95	0.48
1:F:211:LEU:HD22	1:F:246:LEU:HD11	1.96	0.48
1:F:31:LYS:O	1:F:31:LYS:HG3	2.13	0.48
1:A:257:ASP:HB3	1:A:260:TYR:CB	2.44	0.47
1:A:182:SER:HB2	1:A:210:PHE:HB2	1.96	0.47
1:A:494:PRO:HG3	1:C:545:ARG:HB2	1.96	0.47
1:E:17:ILE:HD11	1:E:45:ILE:HD13	1.95	0.47
1:C:339:SER:HB3	1:D:339:SER:HB3	1.96	0.47
1:A:347:ASP:O	1:A:350:VAL:HG12	2.13	0.47
1:B:132:GLU:HB3	1:B:135:LYS:HB2	1.95	0.47
1:F:645:TYR:HA	1:F:685:LYS:HA	1.97	0.47
1:B:182:SER:HB2	1:B:210:PHE:HB2	1.96	0.47
1:A:133:TYR:HB3	1:B:187:TYR:O	2.13	0.47
1:A:247:ILE:N	1:A:247:ILE:HD12	2.29	0.47
1:C:672:LYS:HD2	1:C:678:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:GLN:HE22	1:B:231:GLU:HB2	1.78	0.47
1:F:83:MET:HG3	1:F:101:SER:HB3	1.96	0.47
1:A:278:LEU:HD21	1:E:258:GLN:CG	2.45	0.47
1:D:451:GLY:O	1:D:452:ARG:HG3	2.14	0.47
1:B:83:MET:HG3	1:B:101:SER:HB3	1.95	0.47
1:B:670:VAL:HG22	1:B:680:ALA:HB2	1.97	0.47
1:A:17:ILE:HD11	1:A:45:ILE:CD1	2.45	0.47
1:D:132:GLU:HB3	1:D:135:LYS:HB2	1.97	0.47
1:C:257:ASP:HB3	1:C:260:TYR:CB	2.44	0.47
1:C:132:GLU:HB3	1:C:135:LYS:HB2	1.97	0.47
1:D:610:LEU:HD11	1:D:616:ILE:HD11	1.97	0.47
1:B:247:ILE:HD12	1:B:247:ILE:N	2.30	0.47
1:C:640:PHE:CE2	1:C:644:ILE:HD11	2.49	0.47
1:D:181:ILE:HG13	1:D:209:VAL:HG12	1.97	0.47
1:F:26:PHE:HB3	1:F:165:LEU:HD22	1.95	0.47
1:F:388:ARG:HD3	2:F:840:HOH:O	2.15	0.47
1:B:296:GLU:O	1:B:300:GLU:HG3	2.15	0.47
1:E:293:PHE:O	1:E:299:ARG:HD3	2.15	0.46
1:A:451:GLY:O	1:A:452:ARG:HG3	2.14	0.46
1:A:332:GLU:HG2	1:E:332:GLU:HG3	1.97	0.46
1:E:299:ARG:HG2	1:E:382:ALA:HB2	1.95	0.46
1:D:345:ARG:O	1:D:345:ARG:HG3	2.15	0.46
1:D:37:SER:OG	1:D:40:GLU:HG3	2.14	0.46
1:C:661:ILE:HD11	1:C:693:GLU:CD	2.35	0.46
1:C:183:ARG:HG2	1:C:184:TYR:N	2.31	0.46
1:E:257:ASP:HB3	1:E:260:TYR:CB	2.44	0.46
1:E:555:TYR:HB3	1:E:606:SER:HB3	1.96	0.46
1:D:247:ILE:HD12	1:D:247:ILE:N	2.29	0.46
1:C:643:GLU:CD	1:C:685:LYS:HD3	2.35	0.46
1:E:342:VAL:HG11	1:F:342:VAL:CG2	2.45	0.46
1:B:659:LYS:HE3	1:B:693:GLU:HG3	1.98	0.46
1:D:187:TYR:O	1:F:133:TYR:HB3	2.16	0.46
1:D:211:LEU:HD22	1:D:246:LEU:HD11	1.97	0.46
1:E:175:TRP:CE3	1:E:245:LYS:HG3	2.50	0.46
1:F:183:ARG:HG2	1:F:184:TYR:N	2.30	0.46
1:A:682:ILE:CG2	1:A:684:GLN:HG2	2.46	0.46
1:F:2:ARG:HG2	1:F:47:GLN:OE1	2.16	0.46
1:C:16:VAL:HG13	1:C:20:PRO:HG2	1.97	0.46
1:B:640:PHE:CE2	1:B:644:ILE:HD11	2.51	0.46
1:C:247:ILE:N	1:C:247:ILE:HD12	2.30	0.46
1:D:608:ILE:HD12	1:D:608:ILE:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:670:VAL:CG1	1:B:678:TYR:HB3	2.46	0.46
1:A:187:TYR:O	1:C:133:TYR:HB3	2.15	0.46
1:C:596:HIS:HD2	1:C:598:LEU:N	2.05	0.46
1:C:692:LEU:N	1:C:692:LEU:HD12	2.31	0.46
1:D:228:ARG:C	1:D:230:PRO:HD3	2.37	0.46
1:B:183:ARG:HG2	1:B:184:TYR:N	2.31	0.45
1:A:183:ARG:HG2	1:A:184:TYR:N	2.31	0.45
1:F:3:ILE:HB	1:F:18:GLY:HA2	1.98	0.45
1:C:360:TYR:CE2	1:C:365:ARG:HD2	2.51	0.45
1:D:88:ALA:C	1:D:348:ARG:HD2	2.37	0.45
1:A:26:PHE:HB3	1:A:165:LEU:HD22	1.99	0.45
1:C:183:ARG:O	1:C:185:SER:HA	2.16	0.45
1:E:183:ARG:HG2	1:E:184:TYR:N	2.31	0.45
1:C:360:TYR:CZ	1:C:365:ARG:HD2	2.51	0.45
1:D:182:SER:HB2	1:D:210:PHE:HB2	1.97	0.45
1:C:557:LEU:HD23	1:C:558:TYR:N	2.31	0.45
1:F:242:ARG:HH11	1:F:242:ARG:HG3	1.82	0.45
1:F:247:ILE:N	1:F:247:ILE:HD12	2.31	0.45
1:D:589:LYS:HD2	1:D:589:LYS:HA	1.66	0.45
1:D:609:PRO:HG2	1:D:623:PHE:HE2	1.82	0.45
1:D:687:ARG:HB3	1:D:687:ARG:NH1	2.32	0.45
1:D:8:GLU:HB2	1:D:34:SER:HB2	1.98	0.45
1:A:229:PHE:N	1:A:230:PRO:HD3	2.30	0.45
1:A:258:GLN:CD	1:E:278:LEU:HD21	2.37	0.45
1:A:258:GLN:HG2	1:E:268:GLY:H	1.80	0.45
1:A:646:VAL:HG21	1:A:686:ILE:HD12	1.99	0.45
1:F:451:GLY:O	1:F:452:ARG:HG3	2.17	0.45
1:A:340:LEU:HD13	1:F:340:LEU:HD13	1.99	0.45
1:E:183:ARG:O	1:E:185:SER:HA	2.16	0.45
1:E:451:GLY:O	1:E:452:ARG:HG3	2.15	0.45
1:B:618:TYR:HB2	1:B:652:THR:CG2	2.45	0.45
1:B:451:GLY:O	1:B:452:ARG:HG3	2.17	0.45
1:F:670:VAL:CG1	1:F:678:TYR:HB3	2.47	0.45
1:A:564:LYS:HD3	1:A:564:LYS:N	2.32	0.44
1:B:249:ILE:HA	1:B:318:TRP:HB3	2.00	0.44
1:D:183:ARG:HG2	1:D:184:TYR:N	2.32	0.44
1:D:360:TYR:CE2	1:D:365:ARG:HD2	2.52	0.44
1:C:658:SER:HB2	1:C:693:GLU:O	2.17	0.44
1:C:620:GLU:O	1:C:621:THR:HB	2.18	0.44
1:A:249:ILE:HA	1:A:318:TRP:HB3	2.00	0.44
1:F:38:LEU:HD21	1:F:45:ILE:CD1	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:17:ILE:CD1	1:F:45:ILE:HD13	2.47	0.44
1:E:9:ASN:OD1	1:E:29:GLU:HB2	2.17	0.44
1:B:270:PHE:N	1:D:258:GLN:OE1	2.38	0.44
1:A:670:VAL:HG12	1:A:671:GLU:N	2.32	0.44
1:C:96:ASP:OD1	1:C:97:PRO:HA	2.18	0.44
1:A:640:PHE:CE2	1:A:644:ILE:HD11	2.53	0.44
1:D:241:LYS:CE	1:D:242:ARG:HH12	2.30	0.44
1:B:242:ARG:HG3	1:B:242:ARG:HH11	1.82	0.44
1:D:151:GLU:HA	1:D:151:GLU:OE1	2.16	0.44
1:F:175:TRP:CE3	1:F:245:LYS:HG3	2.53	0.44
1:F:557:LEU:C	1:F:557:LEU:HD23	2.38	0.44
1:F:651:ILE:HD13	1:F:692:LEU:CD2	2.45	0.44
1:E:340:LEU:HD12	1:E:341:PRO:HD2	2.00	0.44
1:E:28:LEU:O	1:E:29:GLU:C	2.55	0.43
1:F:640:PHE:CD2	1:F:644:ILE:HD11	2.53	0.43
1:C:285:PRO:HD2	1:C:288:THR:HG21	2.00	0.43
1:A:22:PRO:HA	1:A:23:PRO:HD3	1.89	0.43
1:C:342:VAL:HG22	1:C:343:GLN:H	1.83	0.43
1:B:332:GLU:CG	1:D:332:GLU:HG3	2.47	0.43
1:C:663:ASP:C	1:C:665:SER:H	2.22	0.43
1:B:183:ARG:O	1:B:185:SER:HA	2.19	0.43
1:A:172:PRO:HG2	1:A:177:PHE:HE1	1.83	0.43
1:C:610:LEU:HD11	1:C:616:ILE:HD11	1.98	0.43
1:B:669:GLN:HA	1:B:669:GLN:OE1	2.19	0.43
1:C:473:PHE:CG	1:C:552:VAL:HG21	2.53	0.43
1:C:637:GLU:OE1	1:C:639:LYS:HE3	2.18	0.43
1:B:88:ALA:O	1:B:348:ARG:HD2	2.19	0.43
1:F:640:PHE:CE2	1:F:644:ILE:HD11	2.54	0.43
1:F:627:ASP:O	1:F:628:ASN:HB3	2.18	0.43
1:F:634:SER:O	1:F:635:SER:C	2.56	0.43
1:F:229:PHE:N	1:F:230:PRO:HD3	2.33	0.43
1:E:249:ILE:HA	1:E:318:TRP:HB3	2.01	0.43
1:F:652:THR:HA	1:F:676:ASN:O	2.19	0.43
1:C:300:GLU:HG2	1:C:385:LYS:HZ1	1.82	0.43
1:C:672:LYS:HD2	1:C:678:TYR:HE1	1.81	0.43
1:F:9:ASN:OD1	1:F:30:GLN:HB2	2.19	0.43
1:F:314:VAL:O	1:F:392:ARG:NH2	2.51	0.43
1:B:133:TYR:HB3	1:C:187:TYR:O	2.18	0.43
1:B:257:ASP:HB3	1:B:260:TYR:HB3	2.00	0.43
1:F:257:ASP:HB3	1:F:260:TYR:HB2	2.01	0.43
1:F:257:ASP:HB3	1:F:260:TYR:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:VAL:HG22	1:B:146:GLU:N	2.34	0.43
1:D:347:ASP:O	1:D:350:VAL:HG12	2.19	0.43
1:C:340:LEU:HA	1:C:340:LEU:HD12	1.81	0.43
1:E:13:TYR:HE2	1:E:36:LYS:HG3	1.79	0.43
1:D:183:ARG:O	1:D:185:SER:HA	2.18	0.43
1:D:215:TYR:C	1:D:215:TYR:CD1	2.92	0.43
1:E:215:TYR:C	1:E:215:TYR:CD1	2.92	0.43
1:D:299:ARG:HG2	1:D:382:ALA:HB2	2.01	0.43
1:F:183:ARG:O	1:F:185:SER:HA	2.19	0.43
1:C:556:LEU:HD23	1:C:557:LEU:N	2.34	0.43
1:C:329:ARG:HB3	1:C:350:VAL:HG22	2.00	0.43
1:E:228:ARG:C	1:E:230:PRO:HD3	2.39	0.43
1:D:567:SER:OG	1:D:593:LYS:HE3	2.18	0.43
1:C:556:LEU:C	1:C:556:LEU:HD23	2.40	0.42
1:B:31:LYS:O	1:B:31:LYS:HG3	2.19	0.42
1:F:215:TYR:CD1	1:F:215:TYR:C	2.93	0.42
1:A:686:ILE:HD13	1:A:690:ILE:CD1	2.43	0.42
1:A:183:ARG:O	1:A:185:SER:HA	2.19	0.42
1:B:172:PRO:HG2	1:B:177:PHE:HE1	1.83	0.42
1:D:96:ASP:OD1	1:D:97:PRO:HA	2.19	0.42
1:B:258:GLN:OE1	1:D:270:PHE:N	2.38	0.42
1:E:285:PRO:HD2	1:E:288:THR:HG21	2.02	0.42
1:C:342:VAL:HG22	1:C:343:GLN:N	2.34	0.42
1:D:257:ASP:HB3	1:D:260:TYR:HB3	2.02	0.42
1:C:257:ASP:HB3	1:C:260:TYR:HB2	2.02	0.42
1:C:604:GLU:HA	1:C:618:TYR:CE2	2.55	0.42
1:E:661:ILE:HD12	1:E:661:ILE:N	2.34	0.42
1:D:609:PRO:CG	1:D:623:PHE:HE2	2.32	0.42
1:A:555:TYR:HB3	1:A:606:SER:HB3	2.01	0.42
1:B:473:PHE:CG	1:B:552:VAL:HG21	2.54	0.42
1:A:93:LYS:O	1:A:94:TYR:HB2	2.19	0.42
1:B:258:GLN:CD	1:D:278:LEU:HD21	2.40	0.42
1:C:249:ILE:HA	1:C:318:TRP:HB3	2.02	0.42
1:F:145:VAL:HG22	1:F:146:GLU:N	2.35	0.42
1:C:589:LYS:HD2	1:C:589:LYS:HA	1.68	0.42
1:D:257:ASP:HB3	1:D:260:TYR:HB2	2.01	0.42
1:E:647:SER:OG	1:E:648:LYS:N	2.52	0.42
1:F:249:ILE:HA	1:F:318:TRP:HB3	2.01	0.42
1:D:94:TYR:CZ	1:E:452:ARG:HG2	2.55	0.42
1:F:340:LEU:C	1:F:342:VAL:H	2.23	0.42
1:D:241:LYS:CE	1:D:242:ARG:NH1	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:LEU:HD23	1:A:548:ASP:HA	2.02	0.42
1:A:375:TYR:N	1:A:376:PRO:HD2	2.35	0.42
1:A:215:TYR:CD1	1:A:215:TYR:C	2.94	0.42
1:C:659:LYS:HD2	1:C:667:GLU:OE2	2.20	0.41
1:B:502:LYS:O	1:B:506:GLU:HG3	2.20	0.41
1:B:257:ASP:HB3	1:B:260:TYR:HB2	2.01	0.41
1:E:257:ASP:HB3	1:E:260:TYR:HB2	2.02	0.41
1:D:241:LYS:HE3	1:D:242:ARG:NH1	2.36	0.41
1:F:589:LYS:HD2	1:F:589:LYS:HA	1.68	0.41
1:A:257:ASP:HB3	1:A:260:TYR:HB2	2.01	0.41
1:F:578:TYR:CE1	1:F:583:GLY:HA2	2.55	0.41
1:D:28:LEU:HA	1:D:28:LEU:HD23	1.90	0.41
1:C:582:ASN:OD1	1:C:582:ASN:C	2.59	0.41
1:C:215:TYR:C	1:C:215:TYR:CD1	2.93	0.41
1:D:555:TYR:HB3	1:D:606:SER:OG	2.20	0.41
1:A:340:LEU:HD12	1:A:341:PRO:HD2	2.01	0.41
1:E:340:LEU:O	1:E:342:VAL:N	2.45	0.41
1:E:22:PRO:HA	1:E:23:PRO:HD3	1.89	0.41
1:C:66:GLY:O	1:C:67:LEU:HB2	2.20	0.41
1:A:627:ASP:O	1:A:628:ASN:CG	2.59	0.41
1:D:213:ILE:HG22	1:D:216:MET:HE3	2.03	0.41
1:A:545:ARG:HB2	1:B:494:PRO:HG3	2.02	0.41
1:D:658:SER:N	1:D:693:GLU:O	2.49	0.41
1:E:589:LYS:HA	1:E:589:LYS:HD2	1.68	0.41
1:F:172:PRO:HG2	1:F:177:PHE:HE1	1.86	0.41
1:B:215:TYR:CD1	1:B:215:TYR:C	2.94	0.41
1:F:74:LEU:HA	1:F:74:LEU:HD12	1.86	0.41
1:A:510:LYS:HE2	1:A:610:LEU:HD13	2.03	0.41
1:C:575:GLY:O	1:C:588:GLY:CA	2.68	0.41
1:F:175:TRP:CD2	1:F:245:LYS:HG3	2.56	0.41
1:A:634:SER:O	1:A:635:SER:C	2.59	0.41
1:F:564:LYS:HG3	2:F:867:HOH:O	2.20	0.41
1:A:542:ASP:O	1:A:546:ILE:HD13	2.20	0.41
1:D:249:ILE:HA	1:D:318:TRP:HB3	2.01	0.41
1:D:483:THR:HG22	1:F:130:LEU:HD22	2.03	0.41
1:D:428:LEU:HD23	1:D:548:ASP:HA	2.03	0.41
1:F:345:ARG:O	1:F:345:ARG:HG3	2.21	0.41
1:C:575:GLY:O	1:C:588:GLY:HA3	2.21	0.41
1:E:510:LYS:HE2	1:E:610:LEU:HD13	2.01	0.41
1:E:682:ILE:HG21	1:E:686:ILE:HD11	2.02	0.41
1:B:187:TYR:HB2	1:B:188:PRO:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:ILE:HA	1:A:609:PRO:HD3	1.89	0.41
1:B:96:ASP:OD1	1:B:97:PRO:HA	2.21	0.41
1:F:579:ASN:HB3	1:F:582:ASN:OD1	2.21	0.41
1:E:340:LEU:HD12	1:E:340:LEU:HA	1.88	0.41
1:D:274:GLU:O	1:D:365:ARG:NH2	2.54	0.41
1:C:257:ASP:HB3	1:C:260:TYR:HB3	2.03	0.41
1:E:632:THR:O	1:E:638:ILE:HA	2.20	0.41
1:F:608:ILE:HA	1:F:609:PRO:HD3	1.80	0.41
1:C:375:TYR:N	1:C:376:PRO:HD2	2.35	0.41
1:D:557:LEU:HD23	1:D:557:LEU:C	2.42	0.41
1:B:38:LEU:HD12	1:B:38:LEU:HA	1.93	0.41
1:C:88:ALA:C	1:C:348:ARG:HD2	2.41	0.41
1:E:257:ASP:HB3	1:E:260:TYR:HB3	2.03	0.41
1:A:175:TRP:CE3	1:A:245:LYS:HG3	2.54	0.41
1:C:145:VAL:HG22	1:C:146:GLU:N	2.36	0.41
1:C:175:TRP:CE3	1:C:245:LYS:HG3	2.55	0.41
1:A:614:GLU:HG2	1:A:648:LYS:HB3	2.03	0.41
1:D:502:LYS:O	1:D:506:GLU:HG3	2.21	0.41
1:E:428:LEU:HD23	1:E:548:ASP:HA	2.02	0.41
1:E:627:ASP:O	1:E:628:ASN:HB3	2.21	0.41
1:D:604:GLU:HA	1:D:618:TYR:CE2	2.56	0.40
1:D:285:PRO:HD2	1:D:288:THR:HG21	2.03	0.40
1:C:183:ARG:C	1:C:185:SER:HA	2.41	0.40
1:F:575:GLY:O	1:F:588:GLY:CA	2.69	0.40
1:C:182:SER:CB	1:C:210:PHE:HB2	2.51	0.40
1:D:596:HIS:HD2	1:D:598:LEU:H	1.69	0.40
1:C:172:PRO:HG2	1:C:177:PHE:HE1	1.86	0.40
1:D:494:PRO:HG3	1:F:545:ARG:HB2	2.02	0.40
1:B:48:GLN:HB3	1:B:49:GLY:H	1.65	0.40
1:D:17:ILE:HD11	1:D:45:ILE:HD13	2.02	0.40
1:D:74:LEU:HD12	1:D:74:LEU:HA	1.86	0.40
1:E:575:GLY:O	1:E:588:GLY:CA	2.69	0.40
1:D:187:TYR:HB2	1:D:188:PRO:HA	2.03	0.40
1:D:4:LEU:HD21	1:D:38:LEU:HD13	2.03	0.40
1:A:301:TRP:CZ2	1:A:305:LEU:HD11	2.57	0.40
1:F:366:VAL:HG12	1:F:367:LYS:O	2.22	0.40
1:C:93:LYS:O	1:C:94:TYR:HB2	2.21	0.40
1:D:145:VAL:HG22	1:D:146:GLU:N	2.36	0.40
1:E:545:ARG:HB2	1:F:494:PRO:HG3	2.03	0.40
1:E:145:VAL:HG22	1:E:146:GLU:N	2.36	0.40
1:A:96:ASP:OD1	1:A:97:PRO:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:555:TYR:HB3	1:E:606:SER:CB	2.52	0.40
1:B:345:ARG:HE	1:C:341:PRO:HA	1.86	0.40
1:F:663:ASP:C	1:F:665:SER:H	2.25	0.40
1:D:542:ASP:O	1:D:546:ILE:HD13	2.21	0.40
1:D:620:GLU:HG2	1:D:634:SER:HA	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	690/693 (100%)	651 (94%)	33 (5%)	6 (1%)	21	36
1	B	690/693 (100%)	653 (95%)	31 (4%)	6 (1%)	21	36
1	C	690/693 (100%)	648 (94%)	35 (5%)	7 (1%)	19	33
1	D	690/693 (100%)	652 (94%)	34 (5%)	4 (1%)	30	48
1	E	690/693 (100%)	649 (94%)	35 (5%)	6 (1%)	21	36
1	F	691/693 (100%)	649 (94%)	34 (5%)	8 (1%)	16	27
All	All	4141/4158 (100%)	3902 (94%)	202 (5%)	37 (1%)	21	36

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	29	GLU
1	C	29	GLU
1	E	29	GLU
1	F	635	SER
1	C	635	SER
1	F	29	GLU
1	A	29	GLU

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Mol	Chain	Res	Type
1	A	635	SER
1	A	688	GLY
1	D	688	GLY
1	F	664	ASP
1	B	635	SER
1	C	688	GLY
1	D	599	PRO
1	E	338	SER
1	E	341	PRO
1	E	688	GLY
1	A	599	PRO
1	C	599	PRO
1	C	647	SER
1	F	30	GLN
1	B	688	GLY
1	F	599	PRO
1	A	49	GLY
1	B	49	GLY
1	C	49	GLY
1	D	49	GLY
1	D	213	ILE
1	E	49	GLY
1	F	49	GLY
1	F	688	GLY
1	A	213	ILE
1	B	213	ILE
1	B	599	PRO
1	C	213	ILE
1	E	213	ILE
1	F	213	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	623/624 (100%)	607 (97%)	16 (3%)	54 79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	623/624 (100%)	604 (97%)	19 (3%)	48	74
1	C	623/624 (100%)	606 (97%)	17 (3%)	52	78
1	D	623/624 (100%)	604 (97%)	19 (3%)	48	74
1	E	623/624 (100%)	602 (97%)	21 (3%)	44	70
1	F	624/624 (100%)	606 (97%)	18 (3%)	50	75
All	All	3739/3744 (100%)	3629 (97%)	110 (3%)	50	75

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	74	LEU
1	A	83	MET
1	A	130	LEU
1	A	165	LEU
1	A	211	LEU
1	A	283	MET
1	A	329	ARG
1	A	392	ARG
1	A	398	LEU
1	A	413	TRP
1	A	426	LEU
1	A	430	LEU
1	A	434	LEU
1	A	463	LEU
1	A	652	THR
1	B	30	GLN
1	B	35	ASN
1	B	41	LEU
1	B	74	LEU
1	B	83	MET
1	B	130	LEU
1	B	165	LEU
1	B	211	LEU
1	B	233	LYS
1	B	283	MET
1	B	329	ARG
1	B	392	ARG
1	B	398	LEU
1	B	413	TRP

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Mol	Chain	Res	Type
1	B	426	LEU
1	B	430	LEU
1	B	434	LEU
1	B	463	LEU
1	B	652	THR
1	C	74	LEU
1	C	83	MET
1	C	130	LEU
1	C	165	LEU
1	C	211	LEU
1	C	283	MET
1	C	329	ARG
1	C	392	ARG
1	C	398	LEU
1	C	413	TRP
1	C	426	LEU
1	C	430	LEU
1	C	434	LEU
1	C	463	LEU
1	C	603	ARG
1	C	628	ASN
1	C	652	THR
1	D	74	LEU
1	D	83	MET
1	D	130	LEU
1	D	151	GLU
1	D	165	LEU
1	D	211	LEU
1	D	283	MET
1	D	329	ARG
1	D	392	ARG
1	D	398	LEU
1	D	413	TRP
1	D	426	LEU
1	D	430	LEU
1	D	434	LEU
1	D	463	LEU
1	D	628	ASN
1	D	652	THR
1	D	659	LYS
1	D	665	SER
1	E	28	LEU

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Mol	Chain	Res	Type
1	E	32	ILE
1	E	41	LEU
1	E	74	LEU
1	E	83	MET
1	E	130	LEU
1	E	165	LEU
1	E	211	LEU
1	E	233	LYS
1	E	283	MET
1	E	329	ARG
1	E	392	ARG
1	E	398	LEU
1	E	413	TRP
1	E	426	LEU
1	E	430	LEU
1	E	434	LEU
1	E	463	LEU
1	E	628	ASN
1	E	630	GLU
1	E	652	THR
1	F	41	LEU
1	F	74	LEU
1	F	83	MET
1	F	130	LEU
1	F	165	LEU
1	F	211	LEU
1	F	231	GLU
1	F	283	MET
1	F	329	ARG
1	F	392	ARG
1	F	398	LEU
1	F	413	TRP
1	F	426	LEU
1	F	430	LEU
1	F	434	LEU
1	F	463	LEU
1	F	628	ASN
1	F	652	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	48	GLN
1	A	343	GLN
1	A	596	HIS
1	B	9	ASN
1	B	30	GLN
1	B	35	ASN
1	B	48	GLN
1	B	343	GLN
1	B	596	HIS
1	C	48	GLN
1	C	343	GLN
1	C	596	HIS
1	C	675	GLN
1	C	676	ASN
1	C	683	ASN
1	D	9	ASN
1	D	48	GLN
1	D	243	ASN
1	D	343	GLN
1	D	596	HIS
1	E	48	GLN
1	E	243	ASN
1	E	343	GLN
1	E	596	HIS
1	E	669	GLN
1	F	48	GLN
1	F	343	GLN
1	F	596	HIS
1	F	675	GLN
1	F	676	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.



## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	691/693 (99%)	-0.06	27 (3%)	43	49	21, 31, 60, 74	0
1	B	691/693 (99%)	-0.06	18 (2%)	59	64	21, 32, 59, 78	0
1	C	691/693 (99%)	0.02	33 (4%)	34	40	22, 32, 66, 84	0
1	D	691/693 (99%)	-0.09	20 (2%)	55	61	20, 30, 54, 78	0
1	E	691/693 (99%)	-0.13	14 (2%)	68	73	18, 30, 50, 80	0
1	F	692/693 (99%)	-0.04	28 (4%)	42	48	19, 31, 63, 83	0
All	All	4147/4158 (99%)	-0.06	140 (3%)	49	55	18, 31, 60, 84	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	49	GLY	7.3
1	B	30	GLN	5.2
1	D	49	GLY	4.9
1	E	30	GLN	4.8
1	A	693	GLU	4.8
1	F	693	GLU	4.6
1	C	687	ARG	4.3
1	C	628	ASN	4.2
1	C	50	ASN	4.0
1	F	29	GLU	4.0
1	C	661	ILE	3.9
1	F	661	ILE	3.9
1	C	667	GLU	3.9
1	E	29	GLU	3.8
1	E	49	GLY	3.8
1	C	49	GLY	3.8
1	C	693	GLU	3.8
1	F	30	GLN	3.7
1	E	50	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	35	ASN	3.7
1	B	344	PHE	3.7
1	F	48	GLN	3.7
1	C	668	ILE	3.6
1	D	50	ASN	3.6
1	F	664	ASP	3.5
1	B	29	GLU	3.5
1	C	29	GLU	3.4
1	B	49	GLY	3.4
1	D	30	GLN	3.4
1	D	346	ASP	3.4
1	D	48	GLN	3.4
1	B	346	ASP	3.4
1	A	664	ASP	3.4
1	F	346	ASP	3.3
1	D	343	GLN	3.3
1	D	669	GLN	3.2
1	C	574	ARG	3.2
1	A	662	VAL	3.2
1	A	346	ASP	3.1
1	B	50	ASN	3.1
1	F	574	ARG	3.1
1	C	669	GLN	3.1
1	B	664	ASP	3.1
1	A	339	SER	3.0
1	D	29	GLU	3.0
1	C	658	SER	2.9
1	A	35	ASN	2.9
1	D	345	ARG	2.9
1	A	48	GLN	2.9
1	B	227	TYR	2.9
1	C	346	ASP	2.9
1	F	343	GLN	2.8
1	E	344	PHE	2.8
1	C	48	GLN	2.8
1	A	393	ASN	2.8
1	F	35	ASN	2.8
1	F	50	ASN	2.8
1	B	628	ASN	2.7
1	E	343	GLN	2.7
1	E	345	ARG	2.7
1	C	659	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	635	SER	2.7
1	D	31	LYS	2.7
1	A	665	SER	2.7
1	F	687	ARG	2.7
1	A	49	GLY	2.7
1	E	35	ASN	2.7
1	D	344	PHE	2.6
1	C	664	ASP	2.6
1	A	343	GLN	2.6
1	E	628	ASN	2.6
1	A	666	LYS	2.6
1	A	661	ILE	2.6
1	D	47	GLN	2.5
1	A	628	ASN	2.5
1	A	669	GLN	2.5
1	C	344	PHE	2.5
1	C	3	ILE	2.5
1	C	593	LYS	2.5
1	C	636	ASN	2.5
1	C	665	SER	2.5
1	F	665	SER	2.5
1	C	670	VAL	2.5
1	F	662	VAL	2.5
1	E	346	ASP	2.5
1	B	48	GLN	2.4
1	B	574	ARG	2.4
1	D	693	GLU	2.4
1	C	47	GLN	2.4
1	F	692	LEU	2.4
1	E	339	SER	2.4
1	F	669	GLN	2.4
1	A	643	GLU	2.4
1	A	655	LYS	2.3
1	C	30	GLN	2.3
1	B	19	GLU	2.3
1	C	102	ILE	2.3
1	A	574	ARG	2.3
1	B	35	ASN	2.3
1	A	587	ASN	2.3
1	E	32	ILE	2.3
1	F	32	ILE	2.3
1	A	687	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	227	TYR	2.3
1	E	48	GLN	2.3
1	C	434	LEU	2.3
1	B	566	GLU	2.3
1	C	343	GLN	2.2
1	C	566	GLU	2.2
1	A	50	ASN	2.2
1	F	344	PHE	2.2
1	C	456	GLU	2.2
1	D	393	ASN	2.2
1	F	658	SER	2.2
1	C	227	TYR	2.2
1	F	666	LYS	2.2
1	D	339	SER	2.2
1	D	32	ILE	2.2
1	C	46	VAL	2.1
1	F	391	HIS	2.1
1	A	344	PHE	2.1
1	D	628	ASN	2.1
1	B	693	GLU	2.1
1	F	667	GLU	2.1
1	A	658	SER	2.1
1	F	342	VAL	2.1
1	F	636	ASN	2.1
1	A	434	LEU	2.1
1	B	28	LEU	2.1
1	A	365	ARG	2.1
1	A	391	HIS	2.1
1	F	635	SER	2.1
1	C	455	ALA	2.1
1	B	340	LEU	2.1
1	F	340	LEU	2.1
1	C	655	LYS	2.1
1	B	345	ARG	2.1
1	E	669	GLN	2.0
1	A	667	GLU	2.0
1	F	345	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.